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TECHNICAL REPORT NO. 549

COMPUTER PROGRAMS FOR A REACTIVE

TURBULENT BOUNDARY LAYER -

AIR VERSION

By B. Bellow

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By B. Bellow

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Antonio Ferri

President

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SUMMARY

Computer programs for the calculation of properties within a reactive compressible turbulent air boundary layer on a flat plate are described. The pressure is constant throughout the boundary layer. The partial differential equations for energy and species mass conservation are solved with arbitrary initial conditions by a finite difference technique. A variable wall temperature boundary condition may be used. The boundary conditions at the edge of the boundary layer are constant with respect to the axial coordinate. The partial differential equations, which describe a two-dimensional diffusing flow may be coupled to a system of equations describing a one-dimensional finite-rate air chemically reacting flow, and hence may be used in the numerical treatment of the two-dimensional reacting boundary layer.

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INTRODUCTION

This report describes an IBM-7094 computer program written in the FORTRAN II language to calculate properties within the turbulent boundary layer, with air chemistry. The analysis is described in Ref. 1. There are three versions of this program, reflecting the substructure, reference, and sublayer hypotheses.

Section I of this report will describe the details common to all versions. Sections II and III will outline those features peculiar to the substructure, reference, and sublayer versions. The major differences in the three versions are the computation of the parameter $d/d\chi(\ln\sigma)$ and the input format for execution on the IBM 7094.

I. TURBULENT BOUNDARY LAYER-AIR CHEMISTRY

A. Basic Equations Used

The program solves two partial differential equations for the dependent variables. stagnation enthalpy ratio, "G", and species mass fractions, " Y_k ", as functions of the two independent variables χ and ψ . These equations are:

$$\frac{\partial G}{\partial \chi} = \frac{\partial}{\partial \psi} \left[\frac{\widetilde{u}}{P_{e}} \cdot \frac{\partial G}{\partial \psi} + \frac{u_{e}^{2}}{2h_{e}} \left(1 - \frac{1}{P_{e}} \right) \widetilde{u} \cdot \frac{\partial (\widetilde{u})^{2}}{\partial \psi} \right] - \left[\psi \cdot \frac{d}{d\chi} \left(\ln \sigma \right) \right] \frac{\partial G}{\partial \psi}$$
(1)

$$\frac{\partial Y_{k}}{\partial X} = \frac{\partial}{\partial \psi} \left[\frac{u}{s_{e}} \frac{\partial Y_{k}}{\partial \psi} \right] - \left[\psi \frac{d}{dX} (\ln \sigma) \right] \frac{\partial Y_{k}}{\partial \psi}$$
 (2)

[k = 1 to 7 in Eq.(2) referring to species $O, N, NO, O_2^-, O_2, N_2, NO^+$]

Explanation of symbols:

Constants in coefficients

P - Prandtl number

S_e - Schmidt number

u - Reference velocity

h - Reference enthalpy

Parameters that are dependent on χ and ψ .

$$\overline{u} = u/u_e$$
 , $G = \frac{h}{h_e}$ (3)

$$\widetilde{\mathbf{u}} = \frac{\overline{\mathbf{u}}}{\overline{\mathbf{u}}_{e}} \left\{ \left(\frac{\overline{\boldsymbol{\xi}}}{\overline{\boldsymbol{\gamma}}} + 1 \right) \boldsymbol{\varphi} \frac{d}{d\chi} \left(\boldsymbol{\xi} \mathbf{n} \boldsymbol{\sigma} \right) \left[\boldsymbol{g}(\boldsymbol{\zeta}, \boldsymbol{\chi}) \right] \right\}$$
(4)

$$\frac{\mathrm{d}}{\mathrm{d}\chi} \left(\ln \sigma \right) = -\frac{1}{\mu_{\mathrm{S}}} \frac{\mathrm{d}}{\mathrm{d}\chi} \left(\mu_{\mathrm{S}} \right) \tag{5}$$

Equations (1) and (2) are converted to difference form and solved by a tri-diagonal matrix method in subroutine STEP. (See Section I-B for method of solution.) The species equation [Eq. (2)] is solved first, followed by the energy equation [Eq. (1)]. A two-dimensional grid of lattice points in the (ζ,ψ) plane is constructed as shown in Fig. 1.

The properties of these mesh are identified by suitable subscripts and superscript as described below:

Subscript, i - mesh points in ψ direction k - scans over 7 species

Superscript, n - mesh points in & direction.

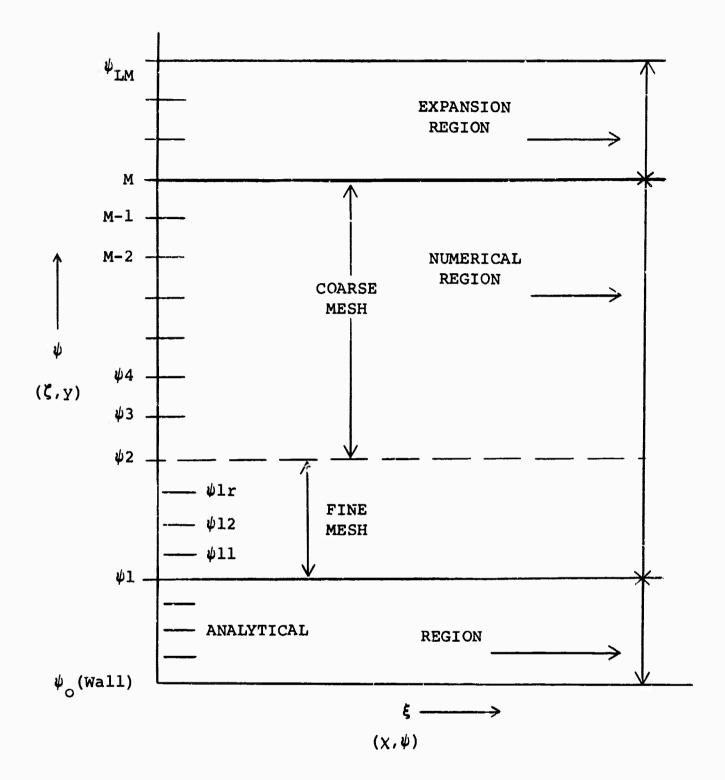


FIG. 1. LATTICE POINTS IN THE (ξ,ψ) PLANE

Subroutine STEP accepts the solutions of the difference equations from the main program at horizontal point $\boldsymbol{\xi}^n$ for all vertical points ψ_i and then steps in the $\boldsymbol{\xi}$ -direction to calculate the species, Y_k , and the enthalpy ratio, G, at point $\boldsymbol{\xi}^{n+1}$ for all ψ_i points. This data is supplied to the main program, for the subsequent calculation of the other thermodynamic properties.

The mesh in the ψ direction (see Fig. 1) is divided into several regions. From the wall at $\psi=0$, an analytical region extends to $\psi=\psi_1$ in which species and enthalpy ratios are found from analytical expressions. For the region $\psi_1<\psi\leq\psi_M$, the difference equations are solved using a fine mesh immediately above the analytical region and a course mesh in the remainder of the region. The fine mesh size was required to provide the necessary numerical accuracy in the solution of the equations. There is an expansion region above $\psi=\psi_M$.

1. Equations for Variables Computed in Analytical Region

$$C1 = \frac{\sqrt{2} \, \varphi}{3\Delta \, \xi} \tag{6}$$

$$GAMMA = -\frac{1}{\varphi^2} \left\{ \frac{u_e^2}{h_e} \left[1 - \frac{1}{P_e} \right] P_e \right\}$$
 (7)

-3

BETA = (C1) (P_e)
$$\{G_o^{n+1} - G_o^n\}$$
 (8)

ALPHA =
$$\frac{\left[G_1^{n+1} - G_0^{n+1}\right]}{\sqrt{\psi_1}} - \sqrt{\psi_1} \quad (GAMMA) \quad . \tag{9}$$

The analytical region, extending from $\psi=0$ (wall) to $\psi=\psi_1$ may be subdivided into an integral number of ψ steps. In this interval, the enthalpy ratios, G_i , and species mass fractions $(Y_k)_i$ are computed from the relations:

$$G_{i}^{n+1} = G_{O}^{n+1} + \sqrt{\psi_{1}} \left\{ ALPHA + \frac{BETA (\psi_{i} - \psi_{1})}{1.0 - \left\{ \frac{d}{d\chi} (\ell_{n} \sigma) \right\} g_{i}} + \sqrt{\psi_{1}} GAMMA \right\}$$
(10)

$$\left(Y_{k} \right)_{i}^{n+1} = \left(Y_{k} \right)_{o}^{n+1} + \frac{(C1) \left(\psi_{i} \right)^{3/2} s_{e} \left\{ \left(Y_{k} \right)_{o}^{n+1} - \left(Y_{k} \right)_{o}^{n} \right\}}{1.0 - \left\{ \frac{d}{d\chi} \left(\ln \sigma \right) \right\} g_{i}} .$$
 (11)

The static enthalpy, h, is found from the stagnation enthalpy and velocity by:

$$h_i = h_e G_i - \frac{1}{2} \overline{u}_i^2 u_e^2$$
 (12)

The mixture temperature T is then obtained from subroutine ENTHLP which computes temperature from static enthalpy and species mass fractions (see Ref. 2).

The mixture molecular weight (WT) $_{\dot{1}}$ and density ratio (RH) $_{\dot{1}}$ are found from

$$(WT)_{i} = \frac{1.0}{\sum_{k} \frac{(Y_{k})_{i}}{M_{k}}}$$
 (13)

$$(RH)_{i} = \frac{(WT)_{i}}{\left(\frac{T_{i}}{T_{e}}\right) / \sum_{k} \frac{(Y_{k})_{e}}{M_{k}}}$$

$$(14)$$

 M_k = molecular weight of k^{th} specie $(Y_k)_e$ = species reference mass fractions (at edge).

The quantities M_k and $(Y_k)_e$ are input data to the problem.

The g_i 's in Eqs. (10) and (11) and the velocity ratios \overline{u}_i are computed in subroutine HERB using the equations of Ref. 1.

The incompressible viscosity "I-VIS" is found from:

$$(I-VIS)_{i} = \widetilde{u}_{i}/\overline{u}_{i} . \qquad (15)$$

If the compressible viscosities "C-VIS" are computed (see Sense Switch 1 Option in Section V), they are found using the relation:

$$(C-VIS)_{i} = \left\langle \frac{(I-VIS)_{i} + \left[\frac{d}{d\chi} (\ln \sigma)\right]g_{i}}{(C/\overline{\mu})^{2}} \right\rangle \left\langle \frac{\tilde{\xi} \rho_{o}}{(\mu)_{o}(\mu)_{i}(\rho)_{i}} \right\rangle. \quad (16)$$

The parameter $(C/\overline{\mu})$ is explained in Sections II and III.

The viscosity μ and the parameter ξ are computed from the relations:

$$\mu_{AIR} = \frac{(3.05 \cdot 10^{-8}) T^{/2}}{T + 111.0}$$
; T in deg. Kelvin (17)

$$\widetilde{\xi} = \frac{\left(\frac{\mu_{o}}{\mu_{s}}\right)^{2}}{1.0-\varphi^{3}\theta \frac{d}{d\chi} (\ln \sigma)}$$
(18)

where φ and θ are functions computed in subroutine HERB (see Ref. 1), and the subscript s which is explained later in Section IIA refers to edge of the sublayer.

2. <u>Difference Equations Used for Numerical Solutions</u>

(a) Generic Form of Difference Equations

The form of the generalized difference equation used to compute species concentrations and energy in the region, $\psi_1 < \psi \leq \psi_M$, is presented in part B of this section and is of the form

$$a P_{i-1} + b P_i + c P_{i+1} = d$$
 (19)

The coefficients of these equations are computed and then the resulting set of linear simultaneous equations are solved in subroutine STEP, first for species and then for the enthalpy ratio. The incompressible eddy viscosities, \tilde{u}_i , are supplied to STEP by subroutine HERB. These viscosities are then corrected at each ψ point for compressibility:

$$\widetilde{u}_{COMP} = \widetilde{u}_{INCOMP} - \overline{u} \left[\frac{d}{dy} (\ln \sigma) \right] (g)$$
 (20)

where u_i and g_i are also obtained from HERB. These compressible \widetilde{u} 's are used in the computation of the a, b, c coefficients in the generic difference Eq. (19) and will be referred to as \widetilde{u} with no subscript. For the species conservation equation, the P_i in the difference equation (19) represents $(Y_k)_i$ and the coefficients are:

$$\lambda_{Y} = \frac{s_{e} (\Delta \psi)^{2}}{\Delta \chi}$$
 (21)

$$a_{i} = \widetilde{u}_{i-\frac{1}{2}}^{n+1} + S_{e}(\Delta \psi)(\psi)_{i} \frac{d}{d\chi} (\ln \sigma)$$
 (22)

$$b_{i} = -\left[\lambda_{Y} + \widetilde{u}_{i+\frac{1}{2}}^{n+1} + \widetilde{u}_{i-\frac{1}{2}}^{n+1}\right]$$
 (23)

$$c_{i} = \widetilde{u}_{i+\frac{1}{2}}^{n+1} - S_{e}(\Delta \psi) (\psi)_{i} \frac{d}{d\chi} (\ln \sigma)$$
 (24)

$$(d_k)_i = -\lambda_Y(Y_k)_i^n$$
 (25)

In the fine mesh region (Fig. 1) the above relations are used from i=ll to i=lr with $\Delta \psi$ being the fine ψ -interval. ψ_{11} is the first fine mesh point above ψ_1 and ψ_{1r} is the last fine mesh point below ψ_2 .

In the coarse mesh region, the above relations are used from i = 3 to i = M with $(\Delta \psi)_{\rm C}$ being the coarse ψ interval.

For ψ_2 ,

$$\lambda_{Y_2} = \frac{S_e(\Delta \psi)_C^2}{2\Delta \chi} \left(1.0 + \frac{1.0}{B} \right)$$
 (26)

B is the total number of fine mesh intervals. Equations (22)-(25) become:

$$a_{2} = B \widetilde{u}_{2-\frac{1}{2}}^{n+1} + \frac{S_{e}}{2} (\Delta \psi)_{c} \psi_{2} \frac{d}{dx} (\ln \sigma)$$
 (27)

$$b_{2} = -\left[\lambda_{Y_{2}} + \widetilde{v}_{2+\frac{1}{2}}^{n+1} + B \widetilde{u}_{2+\frac{1}{2}}^{n+1}\right]$$
 (28)

$$c_2 = \widetilde{u}_{2+\frac{1}{2}}^{n+1} - \frac{s_e}{2} (\Delta \psi)_c \psi_2 \frac{d}{d\chi} (\ln \sigma)$$
 (29)

$$\left(d_{k}\right)_{2} = -\lambda_{Y_{2}}\left(Y_{k}\right)_{2}^{n} \tag{30}$$

For the generic form of the enthalpy ratio difference equations, relations (21)-(24) and (26)-(29) are used with the Schmidt number "Se" replaced by the Prandtl number "Co."

Relation (25) for the right-hand side of (19) is replaced by:

$$d_{i} = -\left[\lambda_{e}(G)_{i}^{n} + (R)_{i} - (R)_{i-1}\right]$$
 (31)

where

$$R_{i} = \left[P_{e} \frac{u_{e}^{2}}{2h_{e}} \left(1 - \frac{1}{P_{e}}\right)\right] \widetilde{u}_{i+\frac{1}{2}} \left[\overline{u}_{i+2}^{2} - \overline{u}_{i+1}^{2}\right]$$
(32)

which is an approximation to the term involving $\frac{\partial}{\partial \psi} \left[\frac{u_e^2}{2h_e} \middle| 1 - \frac{1}{P_e} \middle| \widetilde{u} \frac{\partial (u)^2}{\partial \psi} \right]$ in the energy equation (1). For the λ_e in Eq. (31)

$$\lambda_{e} = \frac{P_{e} (\Delta \psi)^{2}}{\Delta \chi} \tag{33}$$

where the appropriate $\Delta \psi$ is used depending on coarse or fine mesh region. For i=2 Eq. (31) is used for d_2 with λ_e replaced by

$$\lambda_{e_2} = \frac{P_e(\Delta \psi)^2_C}{2(\Delta \chi)} \left(1.0 + \frac{1.0}{B}\right) \tag{34}$$

B is the number of fine mesh intervals.

(b) Boundary Conditions for Difference Equations at $\psi = \psi_1$

At $\psi=\psi_1$ the generic forms of the species and energy equations are replaced by special analytical relations. For the species equation, these are:

$$a_{1s} = 0 (35)$$

$$b_{1S} = \frac{\psi_{1} + (\Delta \psi)_{F}}{2 (\Delta \xi)} + \frac{\widetilde{u}_{3/2}}{(\Delta \psi)_{F} S_{e}} + \frac{1}{A} \left\{ \frac{\psi_{1}}{2 (\Delta \xi)} + \left[\frac{\psi_{1} + (\Delta \psi)_{F}}{2} \right] \left[\frac{d}{d\chi} (\ln \sigma) \right] \left[1.5 (A-1) \right] \right\}$$
(36)

$$c_{1s} = -\frac{\widetilde{u}_{3/2}^{n+1}}{s_e(\Delta \psi)_F}$$
 (37)

$$(d_{k})_{1S} = \left[\frac{\psi_{1} + (\Delta \psi)_{F}}{2 (\Delta \xi)}\right] (Y_{k})_{1}^{n} + \left[\frac{\psi_{1} + (\Delta \psi)_{F}}{2}\right] \left[A-1.0\right] (Y_{k})_{O}^{n}$$

$$+ \frac{1}{A} \left\{\frac{3 \left[1 - \frac{d}{d\chi} (\ln \sigma) \cdot g_{1}\right]}{S_{e} \sqrt{2\psi_{1}} \varphi[\psi_{1} + (\Delta \psi)_{F}]}\right\}$$

$$(38)$$

where $(\Delta \psi)_F$ is the fine mesh interval and

$$A = 1.0 + \frac{S_{e} \sqrt{2} \varphi(\psi_{1})^{\frac{3}{2}}}{[3(\Delta \xi)] [1.0 - \frac{d}{d\chi} (\ln \sigma) \cdot g_{1}]}$$
(39)

After solution of the species equations for the range of ψ from ψ_1 to $\psi_{\underline{M}}$, the species values at the wall are calculated using the following relation:

$$(Y_0^{n+1})_k = \frac{1}{A} [Y_1^{n+1} + (A-1.0)Y_{wall}^n]_k$$
 (40)

The wall enthalpy ratio is found by subroutine ENTHLP from the wall mass fractions $(\mathbf{Y}_0^{n+1})_k$ and the wall temperature.

The energy equation is then solved for the values, G_i , with the following boundary conditions at ψ = ψ_1 :

$$a_{1e} = 0 (41)$$

$$b_{1e} = \frac{\psi_{1} + (\Delta \psi)_{F}}{2(\Delta \xi)} + \frac{\widetilde{u}_{3/2}^{n+1}}{(\Delta \psi)_{F}P_{e}} + \frac{\left(1 - \frac{d}{dX}(\ln \sigma) \cdot g_{1}\right)}{P_{e}\sqrt{2\psi_{1}} \varphi}$$

$$+ \left[\frac{d}{d\chi} (\ln \sigma) \right] \left[\frac{\psi_1 + (\Delta \psi)_F}{4 \sqrt{2}} \right]$$
 (42)

$$c_{1 e} = -\frac{\widetilde{u}^{n+1}}{P_{e}(\Delta \psi)_{F}}$$
 (43)

$$d_{1e} = \left[\frac{\psi_{1} + (\Delta \psi)_{F}}{2(\Delta \xi)}\right] G_{1}^{n} + \left[\frac{-\psi_{1}}{6(\Delta \xi)} + \frac{1 - \left(\frac{d}{d\chi}(\ln \sigma) \cdot g_{1}\right)}{P_{e}\sqrt{2\psi_{1}} \varphi}\right] G_{0}^{n+1} + \left[\frac{\psi_{1}}{6(\Delta \xi)}\right] G_{0}^{n}$$

$$+\frac{1}{2}\frac{u_{e}^{2}}{h_{e}}\left[1-\frac{1}{P_{e}}\right]\frac{\widetilde{u}_{g/2}^{n+1}}{\left(\Delta\psi\right)_{F}}\left[u_{2}^{2}-\left(\frac{\sqrt{2\psi_{1}}}{\varphi}\right)^{2}-\frac{\sqrt{2\psi_{1}}}{\varphi^{2}}\left(1-\frac{d}{d\chi}\left(\ln\sigma\right)\cdot g_{1}\right)\right]$$

$$-\left[\frac{d}{dX} (\ln \sigma)\right] \left[\frac{\psi_{1} + (\Delta \psi)_{F}}{2}\right] \left\{-\frac{g_{O}^{n+1}}{2\sqrt{2}} - \frac{\left(1 - \frac{1}{\sqrt{2}}\right) u_{e}^{2} \left(1 - \frac{1}{P_{e}}\right) 2P_{e}(\psi_{1})^{3/2}}{(2h_{e}) 6(\Delta \xi) \left(1 - \frac{d}{d\chi} (\ln \sigma) \cdot g_{1}\right)}\right\}$$

$$+ \left[\frac{\sqrt{2} \varphi(\psi_1)^{3/2} P_e}{6 \left(\Delta \xi \right) \left(1 - \frac{d}{d\chi} (\ln \sigma) \cdot g_1 \right)} \right] \left[G_o^{n+1} - G_o^n \right]$$
 (44)

3. Trea ment of Psi Expansion Region

To ensure that the solutions satisfy the boundary conditions at the edge, an expansion region is included in the ψ direction.

Before solution of the species equations at the current step, those solutions obtained at $\psi = \psi_{LM}$ for the previous step, are compared with $(Y_k)_e$, which are input. If these comparisons differ by more than a specified tolerance, called EPS, for any one of the species, the values $(Y_k)_e$ are prescribed at an additional ψ point which is added to the mesh (IM is increased by one). The convergence test is:

Is
$$\left| \frac{(Y_k)_{LN} - (Y_k)_e}{(Y_k)_e} \right| \le EPS$$
? (45)

NO - add 1 point to mesh

YES - do not add a point to mesh.

A similar test is performed on the energy equation solution. The test is as follows:

$$Is \left| G_{IM} - 1.0 \right| \leq EPS? \tag{46}$$

NO - add 1 point to mesh

YES - do not add a point to mesh.

At all points in the expansion region, the \widetilde{u} and \overline{u} viscosity parameters are set equal to the values of \widetilde{u} and \overline{u} at $\mathcal{T} = \psi_{M}$. The compressibility correction on \widetilde{u} is not applied in this region.

4. Equations for Parameters Computed after Solution of Difference Equations

Upon obtaining the solutions to the species and energy equations in the numerical region, the main program computes mixture temperature ratios, T_i/T_e , molecular weights, $(WT)_i$, density ratios, $(RH)_i$, and incompressible viscosities, $(I-VIS)_i$, using Eqs. (12) through (15). If desired, compressible viscosities are obtained, using (16). These parameters are printed as output.

The program then computes a value of $\frac{d}{d\chi}$ ($\ln \sigma$) to be used for the next step in the χ direction. The methods used distinguish the substructure, reference, and sublayer versions and will be detailed in Sections II and III.

Having obtained $\frac{d}{dX}$ (ℓn σ), the rhysical coordinate "X" may be found from the coordinate X using

$$x-x_{in.} = \frac{\mu_{o}}{\rho_{o} u_{e}} \int_{x_{in.}}^{x} \frac{1-\varphi^{3} \widetilde{\theta} \left(\frac{d}{dx} (\ln \sigma)\right)}{\left(\frac{\sigma}{\mu} \mu_{o}\right)^{3}} d\widetilde{\chi}$$
(47)

where X_{in} is the initial value of X, and χ_{in} is the corresponding value of X.

Other quantities computed and printed are the heat transfer "Q-DOT," and the skin friction coefficient CF, which are defined by the following relationships:

$$\dot{q} = -\frac{.001285 \ \mu_{o} \left(\frac{\sigma}{\overline{\mu}}\right) \rho_{o} u_{e} h_{e} \alpha}{\sqrt{2} \ \varphi \ P_{e}} \tag{48}$$

$$CF = \frac{2.0 \ \mu_{O} \left(\frac{\sigma}{\overline{\mu}}\right)^{1}}{\varphi^{2} \ T_{O}} \tag{49}$$

The units of \dot{q} are $\frac{BTU}{ft^2-sec}$.

Electron mass fractions are computed from the mass fractions of O_2^- and NO^+ using the following relation:

$$Y_{e^{-}} = \left[\frac{Y_{NO^{+}}}{M_{NO^{+}}} - \frac{Y_{O_{a^{-}}}}{M_{O_{a^{-}}}} \right] / 1820 . \tag{49a}$$

The electron density in particles per cubic centimeter is computed from:

ELECTRON PARTICLE DENSITY =
$$(5.67 \times 10^{26}) (\rho_e^-) (Y_e^-)$$
 (49b)

where $\rho_{e^{-}}$ is the density in slugs/ft³.

5. Finite Rate Chemistry Option

An option has been provided in the program whereby one-dimensional finite rate chemistry reactions are computed using the technique of G. Moretti (Refs. 3 and 4). Using this option, the terms containing the species mass fractions are modified to reflect the coupling of the one-dimensional finite-rate chemistry relations, with the two-dimensional diffusion equations. However, since the correct time step for the chemistry equations is not known until the diffusion equations are solved, a time step iteration is required.

The iteration procedure is as follows:

(1) An approximate ΔX is computed from the previous temperature and species profiles:

$$(\Delta x)^{(1)} = \left[\frac{\mu_{o}}{\rho_{o}\mu_{e}}\right] \left[\frac{1-\varphi^{3}\widetilde{\theta}\left[\frac{d}{dx}(\ln\sigma)\right]}{\left(\frac{\sigma}{\mu}\mu_{o}\right)^{2}}\right] (\Delta x)$$
 (50)

$$(\Delta t)_{i}^{(1)} = \frac{(\Delta x)^{(1)}}{(\rho_{e} u_{e} / \mu_{e}) \overline{u}_{i}}$$
 (51)

- (2) A finite rate chemistry step is performed at each mesh point, ψ_{i} , on the species mass fractions, using the corresponding temperature and density profiles and the " Δ t" profile computed from Eq. (51).
- (3) The diffusion equations are then solved using the chemically modified species profiles.
- (4) New values of $\frac{d}{d\chi}$ (in σ) and c/μ are computed, and then $(\Delta X)^{(2)}$ found, using (50).
- (5) $(\Delta X)^{(2)}$ is compared to $(\Delta X)^{(1)}$. If they are within the specified tolerance, the species and energy solutions are printed as the correct solutions. If the tolerance is not met, steps 2-5 are repeated with the new value of (Δt) . Note that in this case the new value of $\frac{d}{d\chi}$ ($\ell n \sigma$) from step (4) is not used in the left side matrices of the diffusion equations for the next iteration. It is only used to get a new (Δt) approximation for the chemistry calculation.

B. <u>Numerical Methods of Solution of</u> Basic Equations

Partial differential Eqs. (1) and (2) are solved by an implicit second-order central difference method known as the Crank-Nicolson Difference Equation.

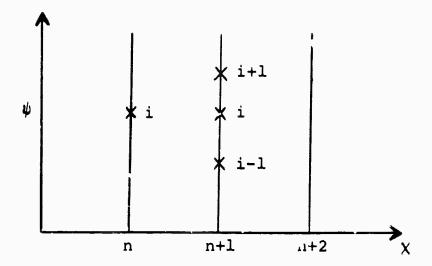


FIG. 2. CRANK-NICOLSON LATTICE POINTS

Assuming a two-dimensional mesh of lattice points with "n" representing the horizontal or χ direction and "i" representing the vertical, or ψ direction, we solve the equation,

$$\frac{\partial P}{\partial X} = \frac{\partial}{\partial \psi} \left[\widetilde{u}(X, \psi) \frac{\partial P}{\partial \psi} \right]$$
 (52)

at a point (n+1), i, assuming known values of P at point n for all values of i. Replace the right side of (52) by a linear relation for the derivative $\frac{\partial [\]}{\partial \psi}$ from i- $\frac{1}{2}$ to i+ $\frac{1}{2}$:

$$\frac{\partial P}{\partial \chi} = \frac{\left(\widetilde{u} \frac{\partial P}{\partial \psi}\right)_{i+\frac{1}{2}}^{n+1} - \left(\widetilde{u} \frac{\partial P}{\partial \psi}\right)_{i-\frac{1}{2}}^{n+1}}{\Delta \psi_{i}} . \tag{53}$$

Each term in the numerator of (53) is approximated in the same manner.

$$\left(\widetilde{u} \frac{\partial P}{\partial \psi}\right)_{i+\frac{1}{2}}^{n+1} = \widetilde{u}_{i+\frac{1}{2}}^{n+1} \left[\frac{P_{i+1} - P_{i}}{\Delta \psi_{i}}\right]^{n+1}$$
(54)

$$\left(\widetilde{u} \frac{\partial P}{\partial \psi}\right)_{i-\frac{1}{2}}^{n+1} = \widetilde{u}_{i-\frac{1}{2}}^{n+1} \left[\frac{P_i - P_{i-1}}{\Delta \psi_i}\right]^{n+1} . \tag{55}$$

The left side of (2) is

$$\frac{\partial P}{\partial X} = \frac{P_i^{n+1} - P_i^n}{\Delta X} \quad . \tag{56}$$

Inserting (54)-(56) into (53)

$$\frac{P_{i}^{n+1}-P_{i}^{n}}{\Delta X} = \frac{1}{(\Delta \psi)_{i}^{2}} \left[\widetilde{u}_{i+\frac{1}{2}} (P_{i+1}-P_{i}) - \widetilde{u}_{i-\frac{1}{2}} (P_{i}-P_{i-1}) \right]^{n+1}. (57)$$

Multiplying both sides of (57) by ($\Delta \psi^2$) and rearranging terms, the difference equation becomes:

$$\widetilde{u}_{i-\frac{1}{2}} P_{i-1}^{n+1} - \left[\frac{(\Delta \psi)_{i}^{3}}{\Delta \chi} + \widetilde{u}_{i+\frac{1}{2}} + \widetilde{u}_{i-\frac{1}{2}} \right] P_{i}^{n+\frac{1}{2}} + \widetilde{u}_{i+\frac{1}{2}} P_{i+1}^{n+1} = -\frac{(\Delta \psi)_{i}^{3}}{\Delta \chi} P_{i}^{n}.$$
(58)

Let

$$a_{i} = \widetilde{u}_{i-\frac{1}{2}}$$

$$b_{i} = -\left[\frac{(\Delta \psi)_{i}^{2}}{\Delta \chi} + \widetilde{u}_{i+\frac{1}{2}} + \widetilde{u}_{i-\frac{1}{2}}\right]$$

$$c_{i} = \widetilde{u}_{i+\frac{1}{2}}$$

$$d_{i} = -\frac{(\Delta \psi)_{i}^{2}}{\Delta \chi} P_{i}^{n}.$$

Then (58) may be written in the form,

1

$$a_{i}P_{i-1}^{n+1} + b_{i}P_{i}^{n+1} + c_{i}P_{i+1}^{n+1} = d_{i}$$
 (59)

Since all P_i for a particular mesh line, n+1, are solved simultaneously for i=1 to ℓ , then we have a set of ℓ equations of type (59) for the unknown P_i 's.

written in matrix form as

[b ₁	C ₁	0	0	O	0	0	$\left\lceil P_1 \right\rceil$		$\left\lceil d_1 \right\rceil$	
a ₂	b₂	C2	0	0	0	0	P ₂		d ₂	
0	a ₃	b_3	C ₃	0	0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	P3	=	đ ₃	
•	•	•	•	•	•		•		•	
0	0	0	0	0	a	b	PL		d _e	

(61)

or

$$AP = D \tag{62}$$

To solve for the unknown P's, the coefficient matrix (called A) is factored into a product of two matrices as follows:

$$[M N] P = D (63)$$

where

The α , β , and γ values of M and N can be evaluated by multiplying M and N and setting the elements of this product matrix equal to the corresponding elements of A. When this is done it is found that

, di

$$\alpha_{i} = a_{i}$$

$$\beta_{i} = b_{i} - \left[\frac{c_{i-1}}{\beta_{i-1}}\right] a_{i}$$

$$\gamma_{i} = \frac{c_{i}}{\beta_{i}}$$
(66)

and $\alpha_1 = a_1 = 0$, $\beta_1 = b_1$, $\gamma_1 = c_1/b_1$.

In (63) let Y = NP. Then since M is a bi-diagonal matrix the transformed unknown column matrix Y can be solved recursively from j=1 to ℓ , as follows:

β_1	0	0	0	0	$\begin{bmatrix} y_1 \end{bmatrix}$	\[\]	1
α₂	β2	0	0	0	Y ₂	đ	2
0	α ₃	$oldsymbol{eta_3}$	0	0	Уз	đ	3
•	•	•	•	•	•	= .	
•	•	•	•	•	•	•	
			α_{ι}	$\boldsymbol{\beta}_{\boldsymbol{\ell}}$	Y	a	e

$$y_1 = d_1/\beta_1$$

$$y_2 = (d_2 - \alpha_2 y_1)/\beta_2$$

$$y_\ell = (d_\ell - \alpha_\ell y_{\ell-1})/\beta_\ell .$$
(67)

At this point, a boundary condition is imposed and \mathbf{y}_{ℓ} is modified such that

$$(Y_{\ell})' = \frac{Y_{\ell}}{1 + \frac{C_{\ell}}{\beta_{\ell}}}$$
 (68)

where $c_{\ell} = \tilde{u}_{e}$.

The solutions P may now be calculated from y_i by sweeping backward from ℓ to 1

$$\begin{bmatrix} 1 & \gamma_{1} & 0 & 0 & 0 & 0 \\ 0 & 1 & \gamma_{2} & 0 & 0 & & \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 1 & \gamma_{\ell-1} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} P_{1} \\ P_{2} \\ \vdots \\ P_{\ell} \end{bmatrix} = \begin{bmatrix} Y_{1} \\ Y_{2} \\ \vdots \\ Y_{\ell} \end{bmatrix}$$
(69)

$$P_{\ell} = Y_{\ell}'$$

$$P_{i} = y_{i} - \gamma_{i} P_{i+1}, \quad i=\ell-1, \ell-2, \ldots 1.$$

II. SUBSTRUCTURE AND REFERENCE HYPOTHESES

A. Calculation of $d/d\chi(\ln \sigma)$

Integrals are computed over the variable "ZETA" (which is a transformed ψ coordinate) for temperature T, species Y_k , and normal coordinate "YCORD." These integrals are:

$$T_{s} = \frac{1}{430} \int_{0}^{430} T_{z} d\zeta$$
 (70)

$$(Y_k)_{s} = \frac{1}{430} \int_{0}^{430} (Y_k)_{\zeta} d\zeta$$
 (71)

where subscript s denotes some mean value across the layer.

As proposed by Coles, the substructure hypothesis is

$$\frac{\sigma}{\overline{\mu}} = \frac{1}{\mu_{\rm S}} \tag{72}$$

where μ_s is the mean value of viscosity in the region $0 \le \zeta \le 430$ and $\overline{\mu}$ is the incompressible viscosity independent of the variable χ .

The normal y-coordinate is obtained using:

YCORD =
$$\frac{\varphi}{\left(\frac{\sigma}{\overline{\mu}}\right)} \rho_{e} \mu_{e} \stackrel{\beta}{\circ} \left(\frac{\rho_{e}}{\rho}\right) d\tilde{z}$$
. (73)

The computing scheme is then as follows: The finite difference equations have been solved for the properties at χ^{n+1} using the value of $\frac{d}{d\chi}$ ($\ell n \sigma$) at χ^n (see Section I, B). (For the first step, $\frac{d}{d\chi}$ ($\ell n \sigma$) is an input value to the program.) Having now the value of μ_s^{n+1} from Eq. (17), the value $\frac{d}{d\chi}$ ($\ell n \sigma$) to be used for the step χ^{n+1} to χ^{n+2} is:

$$\frac{\mathrm{d}}{\mathrm{d}\chi} \left(\ell_{\mathrm{n}} \, \sigma \right) = - \, \frac{1}{\mu_{\mathrm{s}}^{\mathrm{n}}} \left[\frac{\mu_{\mathrm{s}}^{\mathrm{n+1}} - \mu_{\mathrm{s}}^{\mathrm{n}}}{\chi^{\mathrm{n+1}} - \chi^{\mathrm{n}}} \right]. \tag{74}$$

The value of μ_s for n=0 is computed from Eq. (17) using the input temperature and species profiles.

 $\frac{d}{dX}~(\mbox{$\ell n$}~\sigma)$ thus lags the remainder of the solution by one step.

Referring to Fig. 1 of Section I, the fine mesh region for the substructure hypothesis extends over the interval (ψ_1,ψ_2) . The ψ step size between ψ_1 and ψ_2 is therefore

$$(\Delta \psi)_{F} = \frac{\psi_{2} - \psi_{1}}{K} \tag{75}$$

where K is an input number to the program.

The integrals over the logarithmic region [Eqs. (70) and (71)] are found by trapezoidal quadrature in subroutine INTEG, over the values of ζ used in the finite difference mesh. Temperature and species values for the upper limit ζ = 430 are found by linear interpolation.

Since the definition of ζ changes at ζ = 10.6 (see Appendix III, Ref. 1), a special approximation scheme was used for the ζ interval bracketing 10.6. This interval was split into two intervals namely, ζ_1 to 10.6, and 10.6 to ζ_2 , where ζ_1 and ζ_2 are the mesh values of ζ that bracket ζ = 10.6 (see Fig. 3).

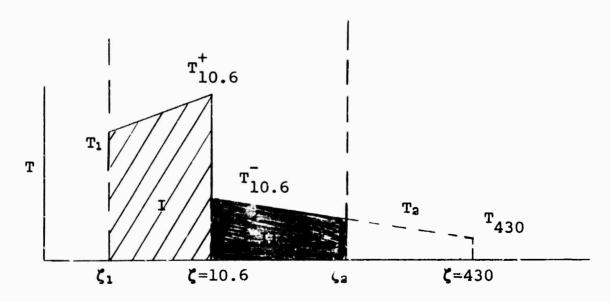


FIG. 3. QUADRATURE DIAGRAM AT $\zeta = 10.6$

A step drop in temperature is imposed at $\zeta = 10.6$, yielding two temperature values, denoted $T_{10.6}^+$ and $T_{10.6}^-$. Two trapezoidal integrations are then performed, the first from T_1 to $T_{10.6}^+$, the second from $T_{10.6}^-$ to T_2 . (See shaded areas I and II in Fig. 3.)

The values of $T_{10.6}^+$ and $T_{10.6}^-$ are obtained as follows:

$$T_{10.6}^{+} = A + B \beta + C \beta^{2}$$
 (76)

where

$$\beta = \varphi/10.6 \tag{77}$$

$$A = T_{O} \tag{78}$$

$$C = \frac{\left[\frac{\overline{T_1}}{\overline{u_1}} - \frac{\overline{T_2}}{\overline{u_2}} + T_O\left\{\frac{1}{\overline{u_2}} - \frac{1}{\overline{u_1}}\right\}\right]}{\overline{u_1} - \overline{u_2}}$$
(79)

$$B = \frac{T_2 - T_0}{\overline{u}_2} - C \overline{u}_2 . \qquad (80)$$

The value of $T_{10.6}^-$ is found from a backward linear extrapolation of the temperatures T_2 and T_{430}^- , where T_{430}^- is the temperature previously found by interpolation at $\zeta = 430$.

B. Modification of Grid Mesh in Normal Direction

The number of grid mesh points in the normal or ψ direction is determined by the value of $\psi_{\mathbf{M}}$, or upper limit of ψ in the numerical region (see Section I). The initial value of $\psi_{\mathbf{M}}$ is known and a ψ spacing of $\psi_{\mathbf{M}}/\mathbf{N}$ is input as $(\Delta \, \psi)_{\mathbf{C}}$. As calculation proceeds in χ direction, $\psi_{\mathbf{M}}$ increases and additional mesh points are added with the $(\Delta \, \psi)_{\mathbf{C}}$. When the total number of these points reaches 2N, the program automatically doubles $(\Delta \, \psi)_{\mathbf{C}}$ and halves the number of points, keeping solution values at every alternate point of the original $\Delta \, \psi$.

For the fine mesh region, whose interval is also doubled, alternate points are kept for the lower half of the region. Points for the upper half of the new fine mesh region are linearly interpolated (see Fig. 4).

For the coarse mesh region, every other point of the original mesh is retained.

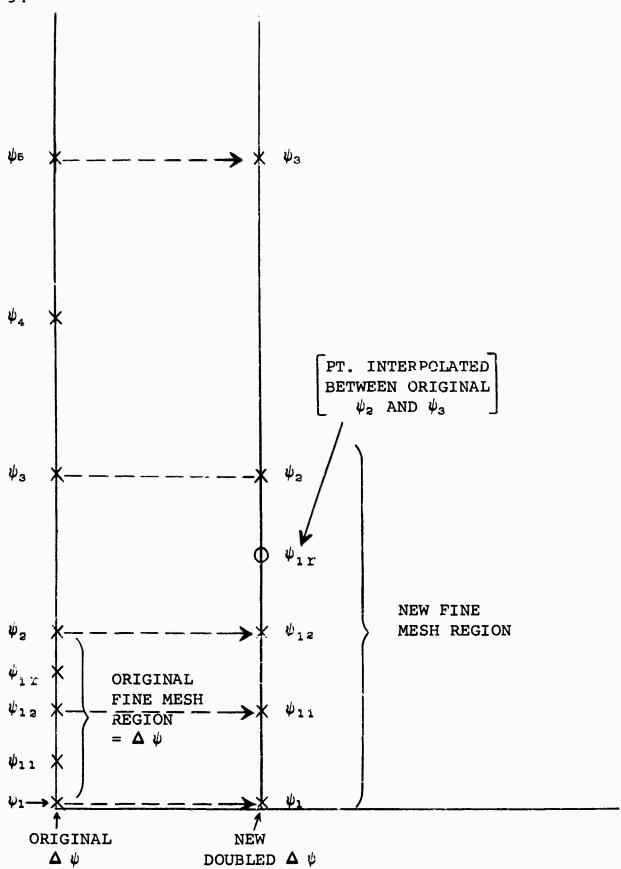


FIG. 4. DOUBLING OF Δ ψ GRID FOR SUBSTRUCTURE HYPOTHESIS

C. Treatment of Wall Chemical Reactions

Finite rate chemistry reactions are computed at all ψ points except at the wall, where an equilibrium chemistry computation is performed.

D. Reference Method Option

When the reference method option is exercised, $\frac{d}{dX}$ ($\ell_{\rm h}$ σ) is set equal to zero. The reference state is still given by the mean substructure values, i.e., $T_{\rm s}$, $(Y_{\rm k})_{\rm s}$, $\mu_{\rm s}$, σ/μ , and YCORD using relations (70), (71), (17), (72), and (73) respectively.

III. SUBLAYER HYPOTHESIS

A. Calculation of $d/d\chi(\ln \sigma)$

The sublayer assumption, proposed by Baronti and Libby, asserts that the Reynolds number based on the height of the laminar sublayer is an invariant of the compressibility transformation. Instead of relation (72) for $\sigma/\overline{\mu}$, one uses the following:

$$\frac{\sigma}{\overline{\mu}} = \frac{1}{10.6} \int_{0}^{56.18} \frac{\rho_{s}}{\rho} \frac{d\widetilde{\psi}}{\sqrt{2\widetilde{\psi}}}$$
 (81)

and

$$\frac{\mathrm{d}}{\mathrm{d}x} (\ln \sigma) = \frac{\frac{\mu_{\mathrm{s}}}{10.6} \int_{0}^{56.18} \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\rho_{\mathrm{s}}}{\rho}\right) \frac{\mathrm{d}\widetilde{\psi}}{\sqrt{2\widetilde{\psi}}} - \frac{\mathrm{d}}{\mathrm{d}x} (\mu_{\mathrm{s}}) \frac{1}{10.6} \int_{0}^{56.18} \frac{\rho_{\mathrm{s}}}{\rho} \frac{\mathrm{d}\widetilde{\psi}}{\sqrt{2\widetilde{\psi}}}}{\mu_{\mathrm{s}}}$$

$$(82)$$

where

$$\frac{d}{dx} \left(\frac{\rho_{s}}{\rho} \right) = \frac{\rho_{s}}{\rho_{e}} \left[\frac{d}{dx} \left(\frac{\rho_{e}}{\rho} \right) - \frac{\rho_{s}}{\rho} \frac{d}{dx} \left(\frac{\rho_{e}}{\rho_{s}} \right) \right]$$
(83)

$$\frac{d}{d\chi} \left(\frac{\rho_e}{\rho} \right) = \frac{\partial}{\partial T} \left(\frac{\rho_e}{\rho} \right) \frac{dT}{dx} + \sum_{k} \frac{\partial}{\partial Y_k} \left(\frac{\rho_e}{\rho} \right) \frac{dY_k}{dx}$$
(84)

$$\frac{d}{dX} \left(\frac{\rho_{e}}{\rho_{s}} \right) = \frac{\partial}{\partial T} \left(\frac{\rho_{e}}{\rho_{s}} \right) \frac{dT}{dX} + \sum_{k} \frac{\partial}{\partial Y_{k}} \left(\frac{\rho_{e}}{\rho_{s}} \right) \frac{dY_{k}}{dX}$$
(85)

$$\frac{\delta}{\delta T} \left(\frac{\rho_{e}}{\rho_{s}} \right) = \frac{1}{r_{s}} \frac{k}{\sum_{k} \frac{(Y_{k}/M_{k})_{s}}{(Y_{k}/M_{k})_{e}}}$$
(86)

$$\frac{\partial}{\partial Y_{k}} \left(\frac{\rho_{e}}{\rho_{s}} \right) = \frac{T_{s}}{T_{e}} \frac{1}{(M_{k})_{s}} \frac{1}{\sum_{k} (Y_{k}/M_{k})_{s}}$$
(87)

$$\frac{d}{dX} (\mu_s) = \left(\frac{d\mu_s}{dT}\right) \left(\frac{dT}{dX}\right)$$
 (88)

$$\frac{d\mu_{s}}{dT} = \left(\frac{3.05 \times 10^{-8} \,\mathrm{T}}{\mathrm{T} + 111.0}\right) \left(1.5 - \frac{\mathrm{T}}{\mathrm{T} + 111.0}\right). \tag{89}$$

The derivatives $\text{d}T/\text{d}\chi$ and $\text{d}Y_k/\text{d}\chi$ are evaluated numerically as:

$$\frac{dT}{d\chi} = \frac{(T)^{n+1} - (T)^n}{\chi^{n+1} - \chi^n}$$
 (90)

$$\frac{dY_{k}}{dX} = \left[\frac{(Y_{k})^{n+1} - (Y_{k})^{n}}{x^{n+1} - x^{n}} \right]_{i}$$
 (91)

In relations (81) to (91), the subscript s refers to parameters evaluated at ψ = 56.18.

The sublayer hypothesis applies to the fine and coarse mesh ψ regions, just as the substructure hypothesis does. However, the fine mesh region now extends from ψ_1 to ψ = 56.18 and can be divided into a prescribed number of intervals.

The normal y-coordinate is still computed from relation (73). As in the substructure hypothesis, calculation of $d/d\chi(\ln\sigma)$ lags the remainder of the solution by one step.

B. Modification of Grid Mesh in Normal Direction

When the criterion for halving the number of intervals in the ψ direction is met (see paragraph 1, Section II, B), the fine mesh ψ points of the original solutions are retained, i.e. the fine mesh region is undisturbed for $0 \le \psi \le 56.18$ ($\psi_{\rm g} = 56.18$).

For the coarse ψ mesh region, 56.18 < $\psi \leq \psi_{\rm e}$, every other mesh point of the original solution is retained.

C. Treatment of Wall Chemical Reactions

Finite rate chemistry reactions are computed at all ψ points. At the wall, a the step is used that is equal to the time step computed at the ψ value closest to the wall. See Eq. (51) for definition of time step (Δ t).

IV. DESCRIPTION OF INPUTS

A. Calculation of Initial Input Data

1. Given Information

The following information must be specified:

- a. External conditions $(u_e, \rho_e, \mu_e, T_e, Y_{ke})$
- $k = 1, \ldots 7$ representing species $O_1N_1NO_1O_2^{-1}, O_2 \cdot N_2$, and NO^+ .
 - b. Wall conditions $(T_0, (Y_k)_0) k = 1, \dots 7$.
 - (1) Initial compressible skin friction coefficient $c_f = \frac{\tau_0}{\rho_e} u_e^2$.
 - (2) Initial compressible Reynolds number based on momentum thickness $R_{\theta} \equiv \rho_{e} u_{e} \theta / \mu_{e}.$
- c. Initial temperature variation with velocity ratio $T(u/u_{\rho})$ through viscous layer.
- d. Initial species mass fraction variation with velocity ratio $Y_k(u/u_e)$ $k=1,\ldots 7$ through viscous layer.

2. Calculation of $\sigma/\overline{\mu}$

As a first step in determining the input data the parameter $\sigma/\overline{\mu}$ must be related to the incompressible skin friction coefficient \overline{C}_f . This procedure varies depending on whether the substructure or sublayer hypothesis is utilized.

a. Calculation of σ/μ According to Substructure Hypothesis

For the substructure hypothesis, take

$$\frac{\overline{\mu}}{c} = \mu_{s} = \mu \left(T_{s} (Y_{k})_{s} \right) \tag{92}$$

where μ_s denotes the viscosity of the mixture evaluated at the temperature T_s , and composition $(Y_k)_s$ where these latter are given by

$$T_{s} = \frac{1}{430} \int_{0}^{430} Td\zeta$$
 (93)

$$(Y_k)_s = \frac{1}{430} \int_0^{430} Y_k d\zeta$$
 (94)

In accordance with items c and d, T and Y_k are known functions of u/u_e . Furthermore, from the Eqs. (AIII-1) through (AIII-6) given in Ref. 1 and the relations

$$\varphi = \sqrt{\frac{2}{C_c}} \tag{95}$$

$$\zeta_{\delta} = \exp\left\{\frac{\varphi - 12.35}{2.43} + 2.03\right\}$$
 (96)

and

$$\frac{\mathbf{u}}{\mathbf{u}_{\mathbf{e}}} = \frac{1}{\varphi} \frac{\overline{\mathbf{u}}}{\mathbf{u}_{\tau}} \tag{97}$$

one can obtain the correspondence between the velocity ratio u/u_e and ζ for any particular value of C_f ;

$$\frac{u}{u_{\varepsilon}} = \frac{u}{u_{e}} \left(\zeta; \ \overline{c}_{f} \right) . \tag{98}$$

Thus the integrals appearing in (93) and (94) can be evaluated (numerically if necessary) and will depend only on a choice of \overline{C}_f . Thus also $\sigma/\overline{\mu}$ will be related uniquely to \overline{C}_f ; i.e.:

$$\frac{\overline{\mu}}{\sigma} = \frac{\overline{\mu}}{\sigma} (C_{\mathbf{f}}) . \tag{99}$$

b. σ/μ According to Sublayer Hypothesis

For the sublayer hypothesis, take

$$\frac{\sigma\mu_{s}}{\overline{\mu}} = \frac{1}{10.6} \int_{0}^{56.18} \frac{\rho_{s}}{\rho} \frac{d\widetilde{\psi}}{\sqrt{2\overline{\psi}}}$$
 (100)

where ρ_s and μ_s denote the density and viscosity of the mixture at $\widetilde{\psi}$ = 56.18. In general, the density is related to the temperature and species by

$$\frac{\rho_{e}}{\rho} = \frac{T}{T_{e}} \left(\sum_{k=1}^{7} \frac{Y_{k}}{M_{k}} \right)_{e} \left(\sum_{k=1}^{7} \frac{Y_{k}}{M_{k}} \right)^{-1}$$
(101)

where the \mathbf{M}_k denote the molecular weights of the individual species and are given. Since the \mathbf{Y}_k and \mathbf{T} are related to the velocity ratio through c and d above we have

$$\frac{\rho_{\epsilon}}{\rho} = \frac{\rho_{e}}{\rho} \left(\frac{u}{u_{e}} \right) . \tag{102}$$

Now relate ρ_e/ρ to $\widetilde{\psi}$ by the relation

$$\frac{u}{u_e} = \frac{\sqrt{2\widetilde{\psi}}}{\varphi} \tag{103}$$

so that, as in the sub-structure case, there can be written formally

$$\frac{\sigma}{\overline{\mu}} = \frac{\sigma}{\overline{\mu}} \ (\overline{C}_{f}) \ . \tag{104}$$

3. Calculation of φ

a. With $C_{\hat{f}}$ given, solve for $\overline{C}_{\hat{f}}$ (by iteration) from the following equation

$$\frac{C_f}{C_f} = \frac{\rho_w - \mu_w}{\rho_e} \frac{\sigma}{\mu} . \qquad (105)$$

b. With R_{θ} given, use Eq. (105) and

$$\frac{R_{\theta}}{R_{\overline{\theta}}} = \frac{1}{\mu_{e}} \frac{\overline{\mu}}{\sigma} \tag{106}$$

$$\overline{C}_{f} = \overline{C}_{f}(R_{\overline{\theta}}) \tag{107}$$

where Eq. (107) is given graphically in Fig. 5. The solution for \overline{C}_{f} is again obtained by iteration.

4. Calculation of φ , ζ_{δ} , ψ_{M}

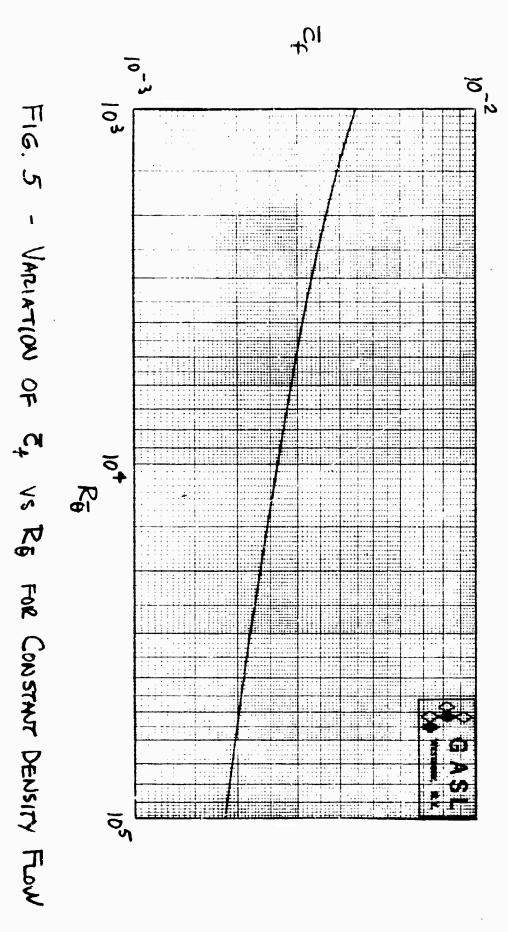
Once an initial value of \overline{C}_f has been obtained the corresponding values of φ and ζ_δ follow from (95) and (96), while ψ_M is obtained from

$$\psi_{M} = -30.81 + 2.43 \zeta_{1} \ln \zeta_{1} + 2.47 \zeta_{1} + (\zeta_{\delta} - \zeta_{1})\varphi + 1.7 \zeta_{\delta}$$
(108)

where $\zeta_1 = 0.131 \zeta_{\delta}$.

5. Calculation of Initial Profiles $T(\psi)$, $Y_k(\psi)$, $G(\psi)$

From the given inputs there is available $T(u/u_e)$ and $Y_k(u/u_e)$. $G(u/u_e)$ is obtained from



$$G = \frac{\sum Y_k h_k}{H_e} + \left(\frac{u}{u_e}\right)^2 \frac{u_e^2}{2H_e}.$$

From the parametric relations

$$\frac{u}{u_e} = \frac{\overline{u}}{\overline{u}} = \text{function of } \zeta$$

$$\psi = \psi(\zeta)$$

given in Appendix III of Ref. 1 there is tabulated the relation

$$u/u_e = u/u_e(\psi)$$

where G, T and Y_k can be obtained as functions of ψ . These are plotted in graphical form from which the desired values corresponding to the previously selected ψ -mesh points ψ_i are read off.

6. Numerical Example (Sublayer Hypothesis)

a. External conditions

$$\rho_e = 1.344 \times 10^{-3} \text{ slugs/ft}^3$$
 $u_e = 2120 \text{ ft/sec}$
 $T_e = 122^{\circ} \text{K}$
 $\mu_e = .4926 \times 1.153 \times 10^{-8} \text{ #/ft-sec}$

$$(Y_6)_e = .232$$
 $(Y_6)_e = 0.768$
 $(Y_k)_e = 0; k = 1,2,3,4,7$
undissociated air

b. Wall conditions

$$T_0 = 306 \text{ °K}$$

$$(Y_k)_0 = (Y_k)_e; k = 1, \dots 7.$$

c. Skin friction coefficient

$$c_{f} = .0013$$
 .

d. Temperature distribution

$$T = T_o + (T_{s_e} - T_o) \frac{u}{u_e} - (T_{s_e} - T_e) \frac{u^2}{u_c^2}$$

(Crocco integral; P_e = 1).

e. Species distribution

$$Y_k(u/u_e) = constant = (Y_k)_e$$
.

Combining e, (101) and (103) gives, using the numerical data

$$\frac{\rho_{\rm e}}{\rho} = 2.51 + 0.22 \frac{\sqrt{2\tilde{\psi}}}{\varphi} - 1.73 \frac{2\tilde{\psi}}{\varphi^2}$$

$$\frac{\rho_{\rm e}}{\rho_{\rm s}} = 2.51 + \frac{2.33}{\varphi} - \frac{194}{\varphi^2}$$

so that from (100)

$$\frac{\sigma \mu_{s}}{\overline{\mu}} = \frac{1}{10.6} \int_{0}^{56.18} \left[\frac{2.51}{\sqrt{2\widetilde{\psi}}} + \frac{0.22}{\varphi} - 1.73 \frac{\sqrt{2\widetilde{\psi}}}{\varphi^{2}} \right] d\widetilde{\psi}$$

$$2.51 + \frac{2.33}{\varphi} - \frac{194}{\varphi^{2}}$$

$$=\frac{2.51+\frac{1.165}{\varphi}-\frac{64.67}{\varphi^2}}{2.51+\frac{2.33}{\varphi}-\frac{194}{\varphi^2}}.$$

Now take an initial guess of $\overline{C}_f = 2x10^{-3}$ so that from (95)

$$\varphi = 22.4$$

for which

$$\frac{\rho_{s}}{\rho_{e}} = 0.451$$

$$\frac{\mu_{\rm S}}{\mu_{\rm R}} = 2.06$$

and

$$\frac{\sigma\mu}{\overline{\mu}} = 1.095.$$

From the given data $\frac{\rho_0 \mu_0}{\rho_e \mu_e} = 1.131$ so that from (105)

$$c_f = \frac{\rho_O \mu_O}{\rho_e \mu_e} \frac{\mu_e}{\mu_s} \frac{\mu_s \sigma}{\overline{\mu}} \overline{c}_f = .0012 < .0013$$
.

A second guess of $\overline{c}_f = .0025$ yields

$$c_f = .00163 > .0013$$
.

A linear interpolation gives as a third guess $\overline{C}_f = .00212$ for which one obtains

$$c_f = .00131 \approx .0013$$

which is the required result.

B. Input Formats for IBM Programs

In this section, the input formats for each of the two program decks - Substructure / Reference Hypothesis, and Sublayer Hypothesis, will be described in detail. Refer to the section on Nomenclature for allied information.

The term "card" refers to the standard IBM data processing card consisting of 12 rows and 80 columns. The term "format" refers to the mode of input. Symbolically, these modes may be defined as follows:

I integer ± XX (no decimal point)

E floating \pm X.XXX \pm YY (YY is the exponent point to the base 10. \pm X.XXX.10 (YY)).

For the E mode, the decimal point may be shifted from the position indicated in the above example and the maximum number of significant figures is governed by the field width assigned for each "word" of data. The plus (+) sign may be omitted in all cases, except for the sign immediately preceding the exponent for the E mode. An additional format is the Hollerith mode which consists of alpha-numerical information, and for our purposes, will be utilized exclusively for an identification input card, which will subsequently be printed as a title at the head of the output listing. It is good practice to "right-adjust" data words within the indicated field; that is, the word must be chifted to the extreme right of the field.

1. Substructure and Reference Hypotheses

CARD	COLUMN	DESCRIPTION	FORMAT
1	1	Punch the number 0	
	2-72	Title information	Н
2	6	Punch the number "1"	
2	14-15	M - Number of coarse mesh points in " ψ " direction, ≤ 40	I
		Total number of species = 7	I
	55	Punch the number "1"	I
	60	Maximum number of iterations on " ΔX " if finite rate chemistry option is requested (≤ 5) [See Eq. (50)]	I
	64-65	Number of fine mesh points in " ψ " direction, \leq 25	I
	69-70	m - Print cycle number - print properties at every $m^{th} \chi$ -step, ≤ 10	I
3	4-5	M - Punch same number as in cols. 14-15, card 2	I
	10	Chemistry option: Punch "1" if finite- rate chemistry requested; punch "0" if no chemistry	I
	15	<pre>"G" input profile option "l" - input temper- ature in ok "2" - input stagnation enthalpy ratios</pre> inputs on 8th set of cards A+1 through C	I
	20	Reference or substructure hypothesis option "0" - substructure hypothesis "1" - reference hypothesis	n I

CARD	COLUMN	DESCRIPTION	FORMAT
4	1-15	" $\Delta \psi$ " for coarse mesh = $(\psi_{M} - \psi_{1})/M$	E
	31-45	Final value of " χ "	E
	61-75	" $arphi_{_{ m O}}$ " - initial $arphi$	E
5	1-15	" $(\zeta\delta)_{_{\mathrm{O}}}$ " - initial $\zeta\delta$	E
	16-30	"HE" - reference stagnation enthalpy (ft ² /sec ²)	E
	31-45	"Δ ξ" - CSI step size	E
	46-60	"DPSY" - " ψ " step size between wall and " ψ_1 "	E
6	1-15	"TROLL" - tolerance for iteration on " Δ X" for chemistry (approx. 0.05) [see Eq. (50)]	E
	16-30	"EPS" - tolerance for adding point to species or energy solution matrix (approx. 0.001) [see Eqs. (45) and (46)]	E
7	1-15	"P " - Prandtl number	E
	16-30	"S _e " - Schmidt number	E
	31-45	" ψ_1 " - first numerical ψ value after wall	Ē
	46-60	"T " - reference temperature (°K)	Е
	61-75	"u = reference velocity (ft/sec)	E
8	1-15	"p " - reference density (slugs/ft ³)	E
	16-30	"#e" - reference viscosity (lb-sec/ft ²)	E
	46-60	Initial value of $\frac{d}{dx}$ (in σ) (substructure version only). Use zero if not krown.	E
	73-75	"SS" - punch 1.0 if $\frac{d}{d\chi}$ ($ln \sigma$) (cols. 50-60) is not zero	E

AND STATE OF THE S

CARD	COLUMN	<u>DESCRIPTION</u> <u>F</u>	ORMAT
9,A	1-15,16-30, 61-75 1-15,16-30	Initial wall species for species 1 to 7. The species are O,N, NO,O2,O3,N3 and NO ⁺ .	E
A+1,A+2B	1-15,16-30, 61-75 1-15, etc.	Values of Y_1 at all fine mean points along initial ψ -mesh line from $\psi=\psi_1$ to point immediately below $\psi=\psi_2$	E
B+1,B+2C	1-15,16-30, 61-75 1-15, etc.	Values of Y_1 at all coarse mesh points along initial ψ -mesh line from $\psi=\psi_2$ to $\psi=\psi_M$, inclusive	E
Y ₂ ther	hrough Y,, and	to "C" for remaining species then for "G" profile. Thus f cards designated A+1	
C+1D	1-15,16-30, 61-75 1-15,16-30	$(Y_k)_e$ for $k = 1, 2,, 7$ (Mass fractions at edge of boundary layer)	E
D+1		Wall temperature function vs. "X" $ (T_W)_1 = A_1 + B_1 X, \text{ for } X \le X_1 $ $ (T_W)_2 = A_2 + B_2 X, \text{ for } X \ge X_1 $	E
	1-15	A ₁ , (°K)	
	16-30	A ₂ , (°K)	,
	31-45	B_1 , $^{\circ}K$ /units of X_1	
	46-66	B ₂ , °K/units of X ₁	
	61-75	$X_i, \rho_e u_e/\mu_e$), where X_i is in feet	
D+2E	1-15,16-30, 61-75	Molecular weights, M _k , for species 1 to 7	E
	1-15,16-30	These values are: $M_1=16.0$, $M_2=14.0$, $M_3=30.0$, $M_4=32.0$, $M_8=32.0$, $M_6=28.0$, $M_7=30.0$	

2. Sublayer Hypothesis

CARD	COLUMN	<u>DESCRIPTION</u>	FORMAT
1	1	Zero	
	2-72	Title information	Н
2	4-5	Number of fine mesh points in " ψ " direction, ≤ 25	I
	9-10	M - Number of coarse mesh points in " ψ " direction, ≤ 40	I
	14-15	TOTAL number of mesh points in " ψ " direction (sum of values in cols. 4-5 and 9-10)	I
	19-20	M (same as in cols. 9-10)	I
	24-25	Punch same as in cols. 14-15	I
	30	"G" input profile option Punch "1" - if temperature in degrees Kelvin are input on 8th set of cards A+1 through C Punch "2" - if stagnation enthalpy ratio (h/h) are input on 8th set of cards A+1 through C	
	35	Punch a "1"	I
	40	Punch a "7"	I
	44-45	m - Print cycle number - print properties at every m^{th} χ -step, ≤ 10	I
	50	Chemistry option: Punch "1" if finite-rate chemistry requested; Punch "0" if no chemistr	

CARD	COLUMN	DESCRIPTION	FORMAT
2	55	Punch "1"	
	60	Chemistry option for (O ₃) "4" - (O ₃) is not included in chemistry reactions "5" - (O ₃) is included in chemistry reactions	I
3	11	Punch "1"	I
	20	Maximum number of iterations on " Δ X" if chemistry option is requested, \leq 5 [see Eq. (50)]	I
4	1-15	" Δ ψ " for coarse mesh region between ψ = 56.18 and ψ = $\psi_{\rm M}$	E
	31-45	" ξ_F " = final value of CSI	E
	61-75	" $arphi_{ m O}$ " - initial $arphi$	E
5	1-15	" $\zeta \delta_{O}$ " - initial ZETA DELTA	E
	16-30	h - reference stagnation enthalpy (ft ² /sec ²)	E
	31-45	" $\Delta \xi$ " - ξ step size	E
	46-60	"DPSY" - Δ ψ for " ψ " between wall and ψ = ψ_1	E
6	1-15	"TROLL" - tolerance for iteration on "\Delta X" if chemistry option is requested, approx05 [see Eq. (50)]	E
	16-30	"ERS" - tolerance on \overline{D} for adding pt. to solution matrix, approx. 0.01 [see Eqs. (45) and (46)]	E
7	1-15	P _e - Prandtl number	E
	16-30	S _e - Schmidt number	E
	31-45	ψ_1 - First numerical " ψ " value above wall	E

CARD	COLUMN	DESCRIPTION	FORMAT
7	46-60	Te - reference temperature (°K)	E
	31-75	u - reference velocity (ft/sec)	E
8	1- 15	<pre>p - reference density (slugs/ft³)</pre>	E
	16-39	<pre>μ_e - reference viscosity</pre>	E
	46-60	Initial value of $\frac{d}{dx}(\ln \sigma)$ (use zero if not known)	<u> 2</u>
	61-75	"SS" - punch "1.0" if cols. 46-60 is not zero or blank	E
9,A	1-15,16-30, 61-75	Initial wall species for species 1 to 7. The species are O.N.NO.	E
	1-15, 16-30	Og, Cg Ng and NO	
A+1, A+2 B	1-15,16-30, 61-75	Values of Y ₁ at all fine mesh points along initial ψ-mesh line	E
	1-15, etc.	from $\psi=\psi_1$ to point immediately below $\psi=56.18$	
B+1;B+2C	1-15,16-30, 61-75	Values of Y_1 at all coarse mesh points along initial ψ -mesh	E
	1-15, etc.	line from $\psi=56.18$ through $\psi=\psi_{M}$	
Ya	through Y7 and	through C for remaining species then for G profile thus there ds designated A+l through C	
C+1 : - D	1-15,16-30	$(Y_k)_e$ for $k = 1, 2, \dots, 7$	E
	61-75 1-15 16-30	(Mass fractions for cdge of boundary layer)	

CARD	COLUMN	DESCRIPTION	FORMAT
D+1		Wall temperature function vs. "X" $(T_W)_1 = A_1 + B_1 X, \text{ for } X \le X_1$ $(T_W)_2 = A_2 + B_2 X, \text{ for } X \ge X_1$	E .
	1-15	A ₁ (°K)	
	16-30	Aa (°K)	
	31-45	B ₁ ^e K/units of X ₁	
	46-60	B_2 $^{\circ}$ K/units of X_1	E
	61-75	$x_1 \cdot (\rho_e u_e / \mu_e)$, where x_1 is in feet	
D+2E	1-15,16-30, 61-75	Molecular weights $M_{f k}$ for species 1 to 7	E
	1-15,16-30	These values are: $M_1 = 16.0$, $M_3 = 14.0$, $M_3 = 30.0$, $M_4 = 32.0$, $M_6 = 28.0$, $M_7 = 30.0$	

V. <u>DESCRIPTION OF OUTPUTS</u>

The output of the program consists of a title page containing program title, names of originator and programmer, a title statement describing the type of computer run, date, etc., and then 17 lines listing the numerical values of all input data.

For each step in the χ direction (CSI), or horizontal coordinate, results are printed in a three page format listing the following information:

Page 1 - The value of "CSI" followed by a seven column table. Each row of the table represents data for a value of "PSI," or vertical coordinate. The columns are, from left to right, (PSI), stagnation enthalpy ratio, G, temperature (TEMP), density (RHO), molecular weight of the mixture, (M), electron mass fraction (ELEC. CON), and electron density in particles per cc.

Page 2 - An eight-column table where the first column contains each value of PSI, while the remaining columns are the mass fractions of each specie. The species are, from left to right, O_1 , O_2 , O_3 , O_4 , O_4 , and O_5 .

Page 3 - A five-column table where the first column contains the vertical "ZETA" variable corresponding to each

"PSI" value. The remaining columns are, from left to right, incompressible viscosity (I-VIS), compressible viscosity (C-VIS), velocity (U-BAR), and the physical vertical coordinate associated with PSI and ZETA, the (Y coordinate) in feet.

Following the data table on page 2 are printed two integers, LE and LS. They indicate the number of PSI values used in the energy and species solutions, respectively.

Following the data table on page 3, except for CSI = 0, are printed the values of X-coordinate, PHI, ZETA DELTA,

DDCHI LOG SIGMA, SIGMA OVER MU-BAR, heat transfer Q-DOT i

BTU per square foot-sec, and CD.

Of the preceding quantities, stagnation enthalpy, density, temperature, velocity, and viscosity are normalized with respect to the input edge conditions.

Examples of the output described herein, appear in Appendix 2.

VI. OPERATING PROCEDURE

The program was written for the IBM 709/90/94 digital computers and uses the IBM FORTRAN II monitor system.

The FORTRAN II monitor system has standard tape designations, which are:

- A2 Standard input tape
- A3 Standard BCD output tape
- Al Systems tape
- A5 Binary tape for restart procedure.

An IOU subroutine is included in the object deck to ensure compatibility with the logical assignment of tapes.

"Checkpoint" Procedure

If a restart option is to be implemented a tape must be mounted on logical unit A5. Depressing sense switch 6 at any time during the course of a run will dump the contents of core memory onto tape A5 and then terminate the run. Tape A5 is dismounted and saved for future use. Tape A3 may then be listed.

To restart at a future time, the binary tape that was saved, is again mounted on logical unit A5 and a small binary object

deck labelled "RESTART," is used as the program deck. The program will read the contents of tape A5 and processing will commence from the point where it was formerly dumped. Processing will continue until Sense Switch 6 is again depressed for a second dump onto tape A5 for a future second restart, etc.

To protect the original information on tape A5, a second tape may be mounted on a unit to be designated as A5 after the original tape has been read by the 7094. The unit with the original tape should be dialed off and the tape dismounted. Core memory will be dumped on the second tape for a future restart.

The program is normally terminated by specifying a value of CSI FINAL on input card 3. When the program has calculated the data for the first value of CSI which is greater than CSI FINAL, the program will automatically process additional sets of input data, or in the absence of such cards, will terminate. A maximum time limit should be specified in the instructions to the operator in this case, in the event of a failure of the program to achieve a value of CSI FINAL.

There are several other program stops, caused by numerical errors, wherein the program will print a code number, and
in some cases an alphabetical statement describing the error.

A list of these error stops is given in Appendix 1. The program will then either process the next data case, or terminate just as in the case of a normal stop at CSI FINAL.

Several options for methods of numerical calculation of the program can be specified on input card 8 and are described in Section IV. There is one option controlled by Sense Switch 1 as follows:

SENSE SWITCH 1

UP - Compressible viscosities are not
 computed and printed. In this case,
 either the number 0 or the values of
 incompressible viscosity are printed,
 the latter for values of PSI greater
 than PSI DELTA.

DOWN - Compressible viscosities are computed and printed.

Sense Switch 1 instructions need be given to the machine operator only if the Sense Switch 1 DOWN option is desired.

See Eqs. (15) and (16) for the equations defining incompressible and compressible viscosities.

NCMENCLATURE

G	stagration enthalpy ratio = H/H e
Н	stagnation enthalpy = $h + u^2/2$
h _i	static enthalpy of species; $h = \sum_{k} h_{k}Y_{k}$
ĝ Ď	effective Prandtl number
ġ	heat transfer per unit time per unit area
s _e	eftective Schmidt number
T	static temperature
ı	mass averaged velocity in axial direction
^M k	molecular weight of species k
x	axial coordinate
2	normal coordinate
Greek Symbols	
δ	boundary layer thickness
ζ	transformed variable defined by Eq. (35) of Ref. 1
η, s	transformed variables defined by Eq. (53) of Ref. 1
$\sigma(x)$, $\eta(x)$, $\xi(x)$	stretching function (see Eq. (15) of Ref. 1)
θ	momentum thickness
μ	laminar viscosity coefficiant
E	kinematic viscosity coefficient

```
transformed variable (see Eq. (47)) of Ref. 1

\rho = \max \text{ density}
\rho \in \text{ eddy viscosity}
\gamma = \sup_{\Psi} |\Psi| = |\Psi|
\text{ stream function defined by Eq. (57) of Ref. 1}
\frac{\text{Subscripts}}{\text{ e}}
\text{ free stream}
```

incompressible state

(")

REFERENCES

- 1. Rosenbaum, H., Compressible Turbulent Boundary Layer with Application to Hydrogen Dumping and Combustion, GASL TR-514, March 1965.
- 2. Thermal Laboratory, Dow Chemical JANAF Interim Thermochemical Tables, December 1960 et seq.
- 3. Moretti, G., A New Technique for the Numerical Analysis of Nonequilibrium Flows, AIAA Journal, Vol. 3, No. 2, February 1955, pp. 223-229.
- 4. De Groat, J. and Abbett, M., A Computation of One-Dimensional Combustion of Methane, AIAA Journal, Vol. 3, No. 2, February 1965, pp. 381-383.

APPENDIX 1

LIST OF FRROR STOPS

APPENDIX 1

LIST OF ERROR STOPS

PRINTED NUMBER	DESCRIPTION OF ERROR
1	An element in Column 2 of species or energy difference equation matrix is equal to zero
6	The number of ψ values given to Subroutine HERB is greater than 149
8	A value of ψ greater than PSI DELTA plus 1/2 DELTA PSI has been computed by Subroutine HERB
9	Subroutine HERB has taken more than 15 itera- tions to compute a value of ZETA
25	No value of "ZETA" is greater than 430
26	Subroutine HERB has computed a value of PSI DELTA less than 1/2 DELTA PSI

APPENDIX 2

SAMPLE OUTPUT OF IBM SHEETS

BLANK PAGE

TURBULENT TRANSPORT ANALYSIS
ORIGINATOR - H. RÜSENBAUM
PROGRAMMER - B. BELLOM
REPERENCE HYPOTHESIS

NET ENEMONE HAT CHIEFE											20000	
COARSE PSI STEP*	5232.00		INITIAL CSI=-0.	•	FINAL	FINAL CSI= 0.12E 10		C31 S	TEP T	CST STEP TOLERANCE=	0.20000 04	5
THE CHIEF		0 2ETA	1 DELTA-	3282.443	I E	0.2240800E 09		CSI STEP=	TEP	0.5000E 02	20	
FINE 'SI STEP"	0.100			TEMP TOL= 0.05000		D-BAR TOL= 1.00E-03		PSI ONE	E E	0.100	9	
DELTA=	0	•										
DD AND TI	1.00	SCHM	MIDT NUMBER# 1.00	:R= 1.00	TE=	1511.10		UE=	407	10248.00		
P-0 E= 0.212000E-03	DE-03	# O E		0.1100000E-05	TRE	300.00		D0 C	וו רספ	00 CHI LOG SIG* -0.		
MAX 202 GF CSI CUTBACKS	UTBACKS=	•	MAX NO.	OF CSI ST	EPS BEFOR	MAX NO. OF CSI STEPS BEFORE DOUBLING=	200					
NO UF SPECIES COARSE PSI POINTS#	ARSE PSI	POINTS=	15	NO. OF COARSE G POINTS"	ARSE G PC	31NTS# 15	NO.	0F F	INE P	NO. OF FINE PSI POINTS=	25	
NC. OF SPECIES=	7	MAX NO.		CF WALL TEMP ITERATIONS=	TIONS-	S PRINI	PRINT CYCLE NUPBER=	NO.	# 62	-		

THE FOLLOWING ARE MOLECULAR WEIGHTS FOR THE SAME SPECIES 1.6000000E 01 1.4000000E 01 3.0000000E 01 3.200000E 01 3.200000E 01 2.800000E 01 3.0000000E 01

THE WALL TEMPERATURE FUNCTION VERSUS X IS 3000-0000+ -0. X FOR X GREATER THAN 0.2400000E 08 3000-3000+ -0. X FOR X GREATER THAN 0.2400000E 08 -

	0	1 7	m ·	4 K	•	~	60 (בַ י		12	13				_	8		2;	17	3 6	54	52		27	28	60 6	2 =	35	33	34	35		37	E (2 4	?
NOP	.0000000E-20	.0000000E-20	7	.0000''00E-20	00C0000E-2	~	.0000000E-20	.0000000E-20	.000000E-20	0000000	-2	.0000000E-20	.0000000E-20	.000000E-20	.000000E-20	?	.0000000E-20	.	.000000E-20	.000000E-20	.000000E-20	.0000000E-20	.0000000E-20			.0000000E-20	.000000E-20	.000000E-20	.00000000-20	.0000000E-20	-2	.0000000E-20	~	.0000000E-20	.0000000E-20	20000000
2	7.6799999E-01 1.7.679999E-01 1.	110	1 10-	7.67999996-01	.679999E-01 1	1 10-35666619	.679999E-01 1	7.6709999E-01 1	.679999E-01 1	.679999E-01 1	1 10-	.6799996-01 1	.6799999E-01 1	.6799996-01 1	·6799996-01 1	.6799999E-01 1	1 10-	100	6799979E-01 1	6799996-01	.6799998-01	5799999E-01 1	1 10-36666619	.6799996-01 1	10-36666629	6799995E-01 1	10	.67999996-01 1	1 10-36660619	7.6799996-01 1	10-	_	10-	10-	7.679999F-01 1	•
05	2.3200000E-01 2.3200000E-01	2.320000E-01	.320000E	2.3200000E-01	.320000E	2.3200000E-01	2.320000E-01	2.3200000E-01	2.320000E-01	2.3200000E-01	2.3200000E-01	2.320000cE-01	3200000	3000000	32000E	2.320000E-01	2.3200000E-01	2.3200000E-G1	2.3200000E-01	2-320000E-01	2-320000E-01	2.3200000E-01	2.3200000E-01	2.3200000E-01	2,3200000E-01	2.3200000E-01	30000056	320000E	.320000E	.320000E	.320000E	2.3200000E-01	2.320000E-01	.320000E.	2.3200000E-01	40 JOOOOOOC+3
MZU																																				
0 7	1.0000000E-20-0.	90	20-	1.00000000E-20-0.	1.000000E-20-0.	9	1.0000000E~20-0.	1.0000000E-20-0.	1.0000000E-20-0.	1.0000000E-20-6.	0	1.0000000E-20-0.	1.0000000E-20-0.	6	1.00000006-20-0.	1.0000000E-20-0.	1.0000000E-20.0.	1.0000000E=20-0.	1.0000000E-20-0.	1.0000000E-20-0:	000000 c-20-	1,0000000E-20-0.	1.0000000E-20-0.	1.0000000E-20-0.	1.0000000E-20-0.	1.0000000E-20-0.	1.000000E-20-0.	1.0000000E-29-0.	1.0000000E-20-0.	1.0000000E-20-0.	0	1.0000000E-20-0.	1.0000000E-20-0.	1.0000000E-20-0.	1.0000000E-20-0.	*^-^2-30000000*T
z	9.9999999E-16	.99999	1-36666666	9.9999399E-16	-36666666.	1-36666666	.999999E-1	9.9999999E-16	-36666666°	1-36666666	1-36666666	66666	-96666666-F	-9666666-I	-9666666.	9666	9666	.999999E-1	9.99999996-16	.999999F-1	-96666666	1-36666666	1-36666666	1-36666666	-36666666.	91~3666666666	00000	66666	-99999996-1	91-3666666666	5	66666*	-36666665°	666666	9. 4999999E-16	アプアアア・
0	9.9999999E-1	1-3666666666666	9.999999E-1	9.9999999E-16	9-96666666-E	1-36666665°6	3666666666	9.99999998-1	1-36 5666 6	9.9999996-1	9-999999E-1	96666666666	9.999999E-1	6.6	9.999999E-1	9.9999999E-1	9.999999E-1	9.9999999E-I	9.99999995-16	9.9999996-1	9-9999999-1	9.999999E-1	1-3666666666	0	9.9999996-1	9.9999998-1		9-999999E-1	9.9999998-1	0	0	0	9.999999E-1	9. 9399999E-1	0	コージケケケケケケ・
PSI	0.000	99E	4.1865999	o «	1.0465000E	1.2557800E	1.4650600E	1.674340GE	1 2.0928999E	2.3021800E	2.5114599E	2.7207400E	2.93001996	3.13930	3.34857896	8 3.5578600E	9 3.7671399E	0 3.9764205E	21 4.1856999E 03	3 4.604259RF	4 4.8135399E	5 5.0228198E	6 5.232099BE	7 1.0464100E	8 1.5696100E	9 2.0928099E		2 3.6624100F	3 4.18560998	4 4.7088099E	35 5.2320099€ 04	5.7552099E	7 6.2784100E	6.8016099E	39 7.3248100E 04	ルケケ CO2 4 5 0 0 0

153	-0- PS1	G	TEMP	A HO	.3	ELEC. (CON. ELEC. DENS.	
0 -	0.	1.6854581E-01		יע ע	2.8836251E 01	8315018E-	1.10891476-02	
-	.0000000E	30000C	821335E	3-3533040E-	.8836251E	.8315018E-2	4273E-0	
7	93799E	-580000085-	.4696514E	2.2373109E-	.8836251E	.8315018E-2	.9255258E-0	
~	36665981.	-3539999E-	.4007493E	2.2723403E-0	3836251E	.8315018E-2	.0025443E-0	
4	6.2793999E	.53699996	-3371617E	2.3056553E-	.8836251E	.8315018E-2	.0759886E-0	
S.	8.3721999E	-9666169	2807579E	2.3360349E-	.8836251E	.8315018E-2	.1428705E-9	
91	1.5455000E	3666618.	2302804E	2.3639095E	.8836251F	.8315018E-2	.2042374E-0	
- 0	1.2557800E	16666416	1849368E	2.3695223E-	.8836251t	.8315018E-Z	2506251E-0	
0 9	1.474.460F	000000000000000000000000000000000000000	34 CU CE	9 0	31670688.	-8315018E-2	. 31 33 360E-0	
. 0	1.88362006	.142999E-	.0702037E	2.4568795E-0	.8836251E	.8315018E-2	89144E-	_
=	2.0923999E	.2029999E-f	.0372815E	2.4769142E-	.8836251E	.8315018E-2	.4530216E-0	-
12	2.3021800E	.2570000E-	.0058233E	2.4963658E-0	.8835251E	.8315018E-2	.4958450E-0	~
13	2. ¢114599E	.306999E-0	7130E	2.5146396E-0	.8836251E	.8315018E-2	.5360754E-0	-
7	2.7237400E	.351999E.0	79094E	2.5329862E-	.8836251E	.8315018E-2	.5764662E-0	_
5	2.9300199E	394999€-0	218526E	2.5498154E-	.8836251E	.8315018E-2	.6135164E-0	~
9 :	3.1393000E	0-75665	968540E	2.5661726E-	.8836251E	.8315018E-2	.6495273E-0	• • •
	3.5483.455	0-05056114	8/240/8E	2.58237265	-8836251E	.8315018E-Z	.6851925E-0	
2 5	34.73.7.8000	0-300000E-0	3441037E	- 200 / 400 /	.8836251E	.8315018E-2	-1195238E-U	~ .
	3-9764200F	.5709999F=0	80492996	2	31670688	1.63120185-25	7860155E-0	
21	4.185699E	-6010000E-0	7844575F	2.6423866F-	8836251F	8315018F-2	8173155F-0	, ~
22	4.3949799E	.6289999	.7540642E	2.6567028E-	.8836251E	8315018E-2	.8488332E-0	117
23	4.6042598E	.6560000E-0	.7446288E	2.6704917	.8836251E	.8315018E-2	0-38681618°	~
54	4.8135399E	·6819999E-0	.7259851E	2.6838540E-	.8836251E	.83;50185-2	.9085075E-D	1.4
25	5.0228196E	.706999E-0	7079868E	2.6968812E-	.8836251E	.8315018E-2	.9372874E-0	1.4
56	5.2320998E	.729999E-0	45E	2.7104425E-	.8836251E	.8315018E-2	.9671431E-0	æ
27	1.04641005	•168999E-0	95E	3.00481725-	.8836251E	315018E-2	.6152202E-0	\sim
2 6	1.5696100E	8.5319999E-01	9783464E	3.357	8836251E	.8315018E-2	.3918142E-0	N 1
200	2.6160100F	1140000E=0	7 Y	-31600061.6-7	31679698	83150185-2 83150185-2	4865412F-0	4 "
31	3.1392100E	339000E-0	0350259E	4.9139423E-	8836251E	315018E-2	.0818232E-0	,
32	3.6624100E	3999E	. 7865437E	5.5974001E-	.8836251E	8315018E-2	.2322891E-0	•
33	4.1856099E	73000E-0	79042CE	6.3329539E-	.8836251L	8315018E-2	.3942241E-0	•
34	4.7088099E	.7880000E-0	080664E	7.1019377E-	.8836251E	3150186-2	.5635188E-0	•
35	5.2320099E	.8740000E	69102E	7.8314642E-	.8836251E	3150185-2	.7241137E-0	177
36	.7552099E	.93300005-0	818815E	8.4619847E-0	.8836251E	3150186-2	.8627403E-0	.,
37	.2784100E	.971000UE	215891E	8.9159211E-0	.8836251E	315018E-2	.9628742E-0	~,
	. 8016099E 0	-990999E-0	886024E	9.1860900E-0	.8836251E	315018E-2	.0223529E-0	· 1
* (324B100E	4440000E-	762664E	9.29138025	.8836251E	8315018E-2	.0455330E-0	-14
•	. 6460049	>	114674	7. 50895 rac=0	• 66 50 £ 51 E	1.8313018E=23	.U494028E-U	•

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CON.	1.3977	.197	5.1971	.071	.007	•	.540	.132	.585	•	•25		.429	.80	.328	.933	.628	.379	.172	.002	.603	.403	.425	.576	.863	.260	. 743	.277	.378	- 900	.349	*	.081	1.2319	.393	. 563	.723	.862	.962	.621	ŏ	2.0488	. 049
ELEC.	.3092252E-1	-2811054E-1	111576-1	-975973CE-2	.4668344E-2	-8931336E-2	.4848264E-2	-9844403E-2	-9883294E-2	.2934132E-2	-7939071E-2	-429071BE-2	-1517826E-2	.3597553E-2	.7014728E-2	.35023636-2	-3133020E-2	.4727365E-2	.1762757E-2	.2085875E-2	.7388369E-2	.345155iE-2	.0228473E-2	.7459936E-2	.514888CE-2	-1204627E-2	.1547803E-2	.C358207E-2	.5861008E-2	.9575541E-2	.8324601E-2		-8310038E-Z	.83100386-2	.8310038E-2	.8310038E-2	.8310038E-2	.8310037E-2	.8310038E-2	.8310038E-2	.8310038E-2	.8310039E-2	.8315016E-2
	5457E 01	127E 0	127E G	966E 0	860E 0	443E 0	868E 0	200E 0	9695	692E C	893E 0	047E C	191E 0	321E 0	434E 0	540E 0	632E 0	217E C	195E 0	867E 0	934E 0	996E G	052E 0	106E 0	155E 0	201E 0	245E 0	87E 0	873E 0	129E 0	221E 0	2	251E 0	252E 0	251E 0	2515 0	252E 0	252E 0	252E 0	252E 0	251E 0	51E 0	251E 0
	.882	. B.B.3	2.8830	.883	.883	.883	2.883	2.803	2.883	2.88	2.88	2.883	2.883	2.883	2.883	2.883	2.8	2.883	2.88	2.883	2.883	2.883	2.883	2.883	2.883	2.883	2.883	2.883	2.883	2.883	2.883	2.8836	2.883	2.88	2.883	2.88	2.883	2.88	2.8	2.883	8	.883	.883
ВНО	5.0356380E-01	.374	.37489	.2420831E-	.2730	-3062565E-	.3365814E-0	.36441025-0	.3899941F-0	.413906	.4363522E-0	.4572807	.477304CE-0	.4967116F-0	-5150174E-	.5332744E-	.5501352E-	-5664963E-	.5826589E	-5982516E-	.6134527E-	.628406	.6426682E-	.6569338E-0	-67C7174E-	.6840826E-0	.6971669E-0	"7106407E-	.0049245E-0	.3576006E-	.7906042E-	96	-9139045E-	- 4973511E-	-328495E-	.1018768E-	.8313522E-0	610438E-0	-9159001E-0	.186090CE-0	.2913	089585E-	.308955
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5 G	1.6886538 :-01	.6040C16E-0	2,6040016E-01	.977531 /E-0	.3238949E-0	.5369801E-0	. (919885E-0	.8139990E-0	.91499; 9E-0	\$0009°1E-9	.07601:1E-0	.14298H8F-0	.2029777E-0	.2570174E-0	.3069466E-0	.3520564E-0	.3949912E-0	.4349684E-0	.4720052E-0	.5069923E-0	.5399808E-0	.5710304E-0	.6009585E-0	.6290147E-0	.4560107E-0	.6819971E-0	.7069146E-0	.7300177E-0	.1689885E-0	.5313923E-0	.8459913E-0	9905E	.3389902E-0	.5239304E-0	.6729904E-0	.7679914E-0	.8739916E-0	.9329934E-0	9.9709942E-01	9909961E-0	.9989976E-0	9	0000000E C
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CC OROINATE	1.2961858E-05 1.2961858E-05	2758143	2.2983808E-03	3.23676336-03	9	4.9670025E-03	7473E-0	6.5712438E-03	.3393542E-0	0889347	8.8223926E-03	9.5412208E-03	1.0246902E-02	1.0940.52E-02	1.16231706-02	1.22956996-02	1.2958802E-02	1.3615076E-02	1.4259087E-02	1.4897296E-02	1.5528165E-02	1.6152083E-02	1.6769375E-02	1.7380399E-02	1.7985469E-02	1.8584765E-02	3.2167290E-02	4.3557432E-02	5.3146771E-02	6.12330736-02	6.8075836E-02	7.3902041E-02	7.8912644E-02	8.32787796-02	8.7149665E-02	9.0659865E-02	9.3927065E-02	9.7050072E-02	w	1.03135375-01
U-848 Y	1.6495042E-02 1.6495042E-02	-36515249	5.10C7361E-01	.3847, JBE-	-36165196-	5.7546577E-01	8892761E-	6.0039969E-01	.1039847E-	926184E-	6.2722306E-01	6.3445001E-01	6.41067586-01	6.4717:206-01	6.52835456-01	6.58119746-01	6.6307215E-01	6.6773219E-01	64E-	6.7630:09E-01	L	æ	.8763201E-	107552E-	6,9437576E-01	6.9754426E-01	7.55974576-01	.0430912E-	.4617506E-	-81300186-	-118882+E-	9.3656770E-01	56375608-	9.71757706-01	9. 8 31 76 E 7E-01	9.911248CE-01	9.9613948E-01	-9882056E-		1.0000000E 00
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ZETA	4.4721359E-01 4.4721359E-01		.9430251E	2605E	.8187280E	.1787707E	2435E 0	2037E	ū	1.3332217E 02	w	w	.70044405	w	1.9390262E 02	.0567844E	.1736308E	6337E 0	.4048525E 0	•5133395E 0	.6331408E 0	.7462974E	.8588462E 0	.97382026 0	.0822493E 0	.1931607E C	.8429866E	0	3106E 0	5590E 0	0	0	.9161680E 0	2.1162743E 03	.3136458E 0	.50909398	2.7032723E 03	7174E 0	896182E C	3.2828251E 03
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N-848 ▼	.6495030E-0	.6495030E-0	.6425125E-0	.1007323E-0	.3847669E-C	5.5916477E-01	.7546535E-0	.8892719E-0	.0039924E-0	.1039802E-	-1926138E-	.272226E-	-3444954E-	.4106710E-	.4717072E-	.5283496E-	.5811925E-	.6307167E-	.6773169E-	-7213215F-	.7630059E-	.8~26041E-	.8403162E-0	.8763149E-0	-9107500E-	.9437525E-0	-9754375E-	7.55973776-01	.0430797E-	.4617372E-	.813º874E-	.1183678E	-3656629E-	9.563743ZE-01	-1170005-	-36/6/168.	.9112415F	-9613906E-	.9882035E-	.9984.82	-36665666 ·	-36666666.	# 1 H d	
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2E1A	4.4721359E-0	4.4721359E-0	2,36482216 0	3.9430251E 0	5.4132505E 0	6.8187280E 0	8.1787707E 0	9.5042435E 0	1.0802037E 0	1.2075883E 0	1.3332217E G	1.4570637E 0	1.5794171E 0	1.7034440E 0	1.820277GE 0	1.9390262E 0	2.0567844E 0	2.1736308E 0	2.2896337E 0	2.46485258 0	2.5193395E U	2.6331408E 0	2.7462974E 0	2.8588462E 0	2.9708202E 0	3.0822493E 0	3.1931607E 0	5.842986	8.3156606E 0	1.0653109E 0	1.2885595E 0	1.5036327E 0	1.7123502E 0	0 30691916*1	2.1162754E 0	2.3136470E 0	2.5090921E 0	2.7032735E G	2.8967185E 0	3.3898192E 0	3.2828259E 0	3.4758030E 0		
	-		C	6	4	5	9	1-	80	6	10	11	12	13	1.4	15	16	! - e-4	18	13	20	21	22	23	24	25	92	27	28	52	30	31	32	33	¥ .	35	36	3.7	38	9	9	41		

DOCHI LCG 31GMA G.

QCOT =-0.32732625E 048TU PER SQUARE FT-SEC

SIGMA OVER MU BAR* 0.43245174E 06

CF= 0.95476717E-03

ACP	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	.2520366-1 .2520366-1 .86273196-1 .26873326-1 .11042646-1 .20500426-1	7.40106295 2.44211415 1.75188885-18 1.28045476-18 1.10447465-18 9.53312505-19 6.27128865-19 6.30510025-19 5.49178125-19 1.06882465-20	00000000000000000000000000000000000000
N 2	.67723666-01 .67813256-01 .67813276-01 .67818876-01 .67849866-01 .67870106-01 .67894926-01	.6791358E-01 .6792020E-01 .6792584E-01 .679362E-01 .679359E-01 .679362E-01	55656-01 55756-01 55756-01 55756-01 55756-01 55756-01 55756-01 55756-01 55756-01	6799986-01 6799986-01 6799996-01 6799996-01 6799986-01 6799986-01 6799986-01 6799996-01
05	3138386E 3155127E 3159240E 316654E 31739556	.31803465 .31818266 .31842116 .31862136		00000000000000000000000000000000000000
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ON	5.9251626E-04 3.9977027E-06 3.9977036E-04 3.8551006E-04 3.1978303E-04 2.4539071E-04 2.4539071E-04 2.4539071E-04		10310976-04 009124346-04 0093264146-05 009366-05 00693126-05 00693126-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05 00601286-05	90512096-07 30952456-08 68810646-09 17950986-10 17950986-12 1794956-12 1794956-15 1791946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15 17781946-15
z	9515949E-0 9359629E-0 9359629E-0 2326420E-0 0241518E-0 9353869E-0	.14703065 .16218296 .3291426 .3291426 .03008126 .77559846 .56*48806 .356*48806	1003400 1003400 3381330 3381330 303863 303863 303863 303868 30388	2402. 2405. 24
0	2.9975647E-0 2.3550179E-0 2.3550179E-0 2.0199007E-0 1.6796820E-0 1.2959334E-0 1.16693309E-0	4.0347215 4.0347316 9.0832675 6.4590685 7.90780595 7.41313205 6.97667655 6.57156925 6.57156925	5.8939305 5.8939405 5.8939405 5.8939405 6.8236416 4.60386416 4.60348356 3.8663196 1.45355496 1.148586 1.1485886	2.06973446-0 2.626877:E-0 2.62877:E-0 1.8413946E-1 1.786217E-1 8.576860E-1 1.698817E-1 6.9255357E-1 5.024554E-1 1.0011850E-1
	000000	0000000	000000000000000000000000000000000000000	0000000000
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TOKEULEST THANSPORT ANALYSIS
ORIGINATOR - H. ROSEUBAUM
PROGRANMER - B. RELLON

CHECK RUN OF ATH IN: UT 6/23/65 SUBLAYER HYPOTHESIS

COARSE PSI STEP=	1051.66	THITIAL CSI=+0.	FINAL CST= 0.35E 06	CSI STEP TOLERANCES 0.20000E 04
INITIAL FILE	24.25400	2E.TA DELTA= 1012.480 HE= 0.3577980E 07	HE= 0.3577980E 07	CSI STEP= 0.1000F 86
FINE PSI STEP= DELTA=	0.100	* 21	L 1EMP TOL= 0.05000 P-PAP TOL= 1.00E-03	PSI ONFE 0+100
94ANDTL NUMBER= 1.00 840 E= 0.422300E=03	1.U0 E-03	SCHMIDT NUMNER= 1.00 MU E= 0.1758766E-06	TE= 121.63 TR= 500.80	UE= 2138.45 DD CHI LOG SIG= -0.

50 MAX HO. OF CSI STEPS REFORE DOUBLING= 500 20 NO. OF COARSE G POINTS= 20 NO. OF FINE PSI POINTS= PPINT CYCLE NUMBER= ijΛ MAX NO. OF WALL TEMP ITERATIONS= MAX 1.0. OF CSI CUTBACKS= 5 NO OF SPECIES COAKSE PSI POINTS= 7 NO. OF SPECIES=

THE WALL TEMPERATURE FUNCTION VERSUS X IS
305.81400+ -7. X FOR X LESS THAN 0.24400000E 08
305.81400+ -0. X FOR X GREATER THAN 0.24400000E 08

THE FOLLOWING ARE MOLECULAR WEIGHTS FOR THE SAME SPECIES
1.6000000E 01 1.4000000E 01 3.0000000E 01 3.200000E 01 2.8000000E 01 3.0000000F 01

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	1.69h5187E-05			1.57984936-04	1.8197612E-04	2.03037756-04	2.2199946E-04	2.3935710E-04	2.5543520E-04	2.7046012E -04	2.8459725F-04	2.9797189E-04	3.106H172E-04	3.22804616-04	3.3440388E-04	3.45531755-04	3.5623204E=04	3.5654197E-04	3.76493375-04	3.8611376E=04	3.9542714E-04	2.8184524E=03	4.6492226E=03	6.2575936E-03	7.6934377E-03	8.9860556E-03	1.0159059E-02	1.1231812E-02	1.2220495E-02	1.313A839E-02	1.3998657E=U2	1.48102255-02	1.5582529E=02	1.63234695-02	1.70394926-02	1.77381691-02	1.8423245E-02	1.9099629E-02	1.9770004F-02	2.043/742E-02
1.84387558-02	1.84347565-02	9.9364195E-02	1.3930721E-01	1.70116895-01	1.961453RE=01	2-19103332E-01	2.3987397E-01	2.5P9R412E-01	2.7677705F-01	2.9349495E=01	3.0030979E=01	3.2435443E+01	3.38731546-01	3,5252278E-01	3.6570443E-01	3.78601145-01	3.909RR59E-01	4.02995456-01	4.1465478E-01	4.2590512F=01	4.3704130E-01	n.4870430E-01	7.05349506+01	7.4944B25F-01	7.889r :56E=01	8.24022095-01	8.5504474E-01	A.8230258E-01	9.05993P6E=01	9.263A130E=01	9.43701825-01	9.5818156E=01	9.7004398F-01	9.79513325-01	7.86A1927F-01	9-920172E-01	9.9591581E=01	9.98236856-01	0.90465305=01	10-3651£666
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